# WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Monday, September 25, 2006

| Hide? | Set Name | Query | Hit Count |
|---|---|---|---|
| | | *DB=PGPB; PLUR=YES; OP=ADJ* | |
| ☐ | L2 | (diarylfuran).clm. | 1 |
| ☐ | L1 | (dicatioic diarylfuran).clm. | 0 |

END OF SEARCH HISTORY

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* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *
* * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:03:45 ON 25 SEP 2006

=>  file reg
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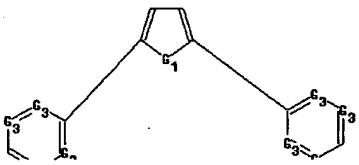

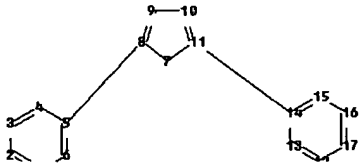

```
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17
chain bonds :
5-8  11-14
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-11  8-9  9-10  10-11  12-13  12-17  13-14  14-
15  15-16  16-17
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-8  7-8  7-11  8-9  9-10  10-11  11-14  12-13  12-17
13-14  14-15  15-16  16-17
isolated ring systems :
containing 1 : 7 : 12 :


G1:O,S,N

G2:O,S,N

G3:C,O,S,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom



L1      STRUCTURE UPLOADED

=> dis l1
L1 HAS NO ANSWERS
L1              STR
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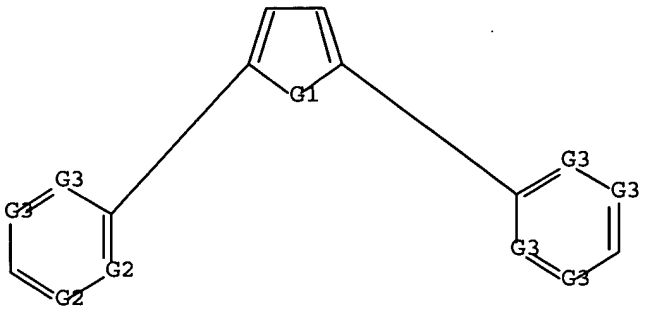


G1 O,S,N
G2 O,S,N
G3 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sam
L2             0 SEA SSS SAM L1

=> s l1 full
L3             6 SEA SSS FUL L1

=> file caplus

=> s l3
L4             6 L3

=> s l4 and pd< nov 2002
      22740598 PD< NOV 2002
                  (PD<20021100)
L5             4 L4 AND PD< NOV 2002

=> dis l5 1-4 bib abs hitstr

L5   ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2000:790486  CAPLUS Full-text
DN   133:335249
TI   Preparation of pesticidal triazine derivatives
IN   Steiger, Arthur; Zambach, Werner; Jeanguenat, Andre; Eberle, Martin; Trah,
     Stephan; Farooq, Saleem
PA   Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft
     m.b.H.
SO   PCT Int. Appl., 101 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     --------------      ----   --------    --------------------    --------
PI   WO 2000066568        A1    20001109    WO 2000-EP3921          20000502 <--
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
             SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
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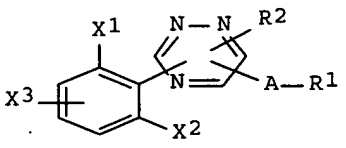
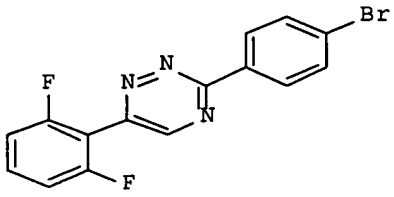
| | | | | | |
|---|---|---|---|---|---|
| | RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2368582 | AA | 20001109 | CA 2000-2368582 | 20000502 <-- |
| | EP 1175410 | A1 | 20020130 | EP 2000-922671 | 20000502 <-- |
| | EP 1175410 | B1 | 20051207 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY | | | | |
| | BR 2000010294 | A | 20020213 | BR 2000-10294 | 20000502 <-- |
| | JP 2002543191 | T2 | 20021217 | JP 2000-615599 | 20000502 |
| | AU 762755 | B2 | 20030703 | AU 2000-42986 | 20000502 |
| | RU 2252217 | C2 | 20050520 | RU 2001-132322 | 20000502 |
| | AT 312085 | E | 20051215 | AT 2000-922671 | 20000502 |
| | ES 2254165 | T3 | 20060616 | ES 2000-922671 | 20000502 |
| | ZA 2001008943 | A | 20020625 | ZA 2001-8943 | 20011030 <-- |
| | US 2003036544 | A1 | 20030220 | US 2001-6954 | 20011205 |
| | US 6723720 | B2 | 20040420 | | |
| PRAI | CH 1999-832 | A | 19990504 | | |
| | WO 2000-EP3921 | W | 20000502 | | |
| OS | MARPAT 133:335249 | | | | |
| GI | | | | | |




I



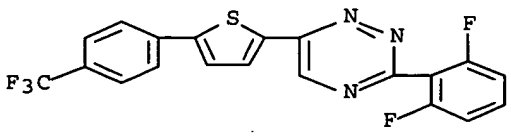

II

AB The title compds. [I; R1 = (un)substituted aryl, heteroaryl; R2 = H, OH, halo, etc.; A = a single bond, alkylene, O, O(alkylene); X1 = halo, CN, NO2, etc.; X2, X3 = H, halo, CN, etc.] which are suitable especially in the control of pests in agriculture and stored goods and also in the keeping of domestic animals, were prepared Thus, treatment of 2,6- difluoroacetophenone with Br2 in the presence of AlCl3 in CHCl3 followed by reaction of the resulting 2-bromo-1-(2,6-difluorophenyl)ethanone with 4-bromobenzoic acid hydrazide in the presence of AgOAc in dimethoxyethane afforded triazine II. Biol. data for compds. I was given.

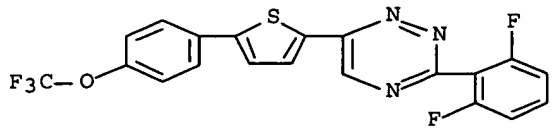
IT 304671-84-9P 304671-86-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pesticidal triazine derivs.)

RN 304671-84-9 CAPLUS

CN 1,2,4-Triazine, 3-(2,6-difluorophenyl)-6-[5-[4-(trifluoromethyl)phenyl]-2-thienyl]- (9CI) (CA INDEX NAME)

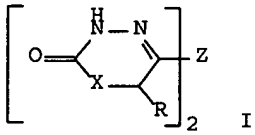


RN 304671-86-1 CAPLUS
CN 1,2,4-Triazine, 3-(2,6-difluorophenyl)-6-[5-[4-(trifluoromethoxy)phenyl]-2-thienyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1990:235248 CAPLUS Full-text
DN 112:235248
TI 1,4-Bis(3-oxo-2,3-dihydropyridazin-6-yl)benzene analogs: potent phosphodiesterase inhibitors and inodilators
AU Coates, William J.; Prain, H. Douglas; Reeves, Martin L.; Warrington, Brian H.
CS Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK
SO Journal of Medicinal Chemistry (1990), 33(6), 1735-41
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 112:235248
GI



I

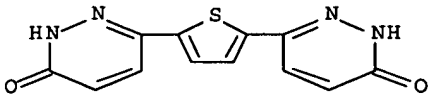
AB The title compds. I (R = H, Me; X = S, CH2; Z = 1,4-, 1,3-C6H4, 2,5-thienyl, 4-C6H4C6H4-4') were prepared from bis(alkanoyl)benzenes by conversion to γ-keto acids and treatment with N2H4. I were evaluated for inhibition of low Km, cAMP-selective, cGMP-inhibited phosophodiesterase (PDE III) and hemodynamic activity. The most potent PDE III inhibitor was I (R = Me, X = CH2, Z = 1,4-C6H4) which also retained the greatest inotropic and vasodilator potency. PDE III inhibitory potency is associated with overall planar topol. of the phenylpyridazinone moiety and the presence of two critically separated electroneg. centers. The generally higher level of PDE III inhibitory potency of I relative to 6-(4-substituted-phenyl)pyridazin-3(2H)-one derivs. (e.g. Sicar, I; et al., 1987, Moos, W.H.; et al., 1987) derives from a closer to optimal separation of two interacting points in the inhibitor mol. achieved through the more extended bis(azinone) structure. Correlation between the

pharmacol. and PDE III inhibitory activities of I provides addnl. evidence for PDE III being an important mediator of inodilator action.

IT 112127-79-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, ionotropic, vasodilator, and phosphodiesterase inhibiting activities of)

RN 112127-79-4 CAPLUS

CN 3(2H)-Pyridazinone, 6,6'-(2,5-thiophenediyl)bis- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:48712 CAPLUS Full-text

DN 108:48712

TI Strategic approaches to drug design. II. Modeling studies on phosphodiesterase substrates and inhibitors

AU Davis, A.; Warrington, B. H.; Vinter, J. G.

CS Smith Kline and French Res., Welwyn/Herts., AL6 9AR, UK

SO Journal of Computer-Aided Molecular Design (1987), 1(2), 97-119
CODEN: JCADEQ; ISSN: 0920-654X

DT Journal

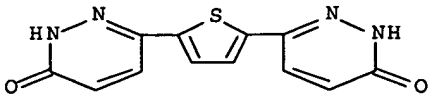
LA English

AB Computational chem. and mol. graphics were combined with both phys. and biol. data to study the interactions of the cat ventricle phosphodiesterase enzyme with the natural substrates cAMP and cGMP and synthetic inhibitors. Specific binding points (defined by points at which the electrostatic interaction of a proton with the target are most stable) were used to give a consistent picture of the binding requirements of both nonspecific and specific inhibitors. These points are situated on or beyond the van der Waals surface and broadly consist of: (a) a single, large point corresponding with an anionic group and probably representing a primary link; (b) a variable set of points associated with the purine of the natural substrate which are likely to represent the secondary binding area and which are able, in appropriate combination with (a), to define specificity; and (c) a 3rd point which ( by hydrophobic interaction) can further affect potency by its (chiral) influence. The complementary study by lone-pair construction and regression anal. reached essentially the same working rules for structure-activity and provided quant. support for the hypothesis. It is notable that structural overlay in this particular case seems to be of less significance than electronic overlay. Indeed, structural comparisons have been misleading at times. The main driving forces for recognition and orientation are undoubtedly the coulombic interactions which were the subject of these studies. However, steric influences play their part in the bound state. Compds. designed to access the more effective N(1) site demonstrated by these studies were found to show the expected high potency.

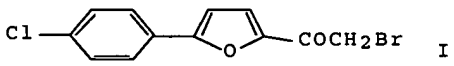
IT 112127-79-4
RL: BIOL (Biological study)
(cyclic nucleotide phosphodiesterase inhibition by, structure in relation to)

RN 112127-79-4 CAPLUS

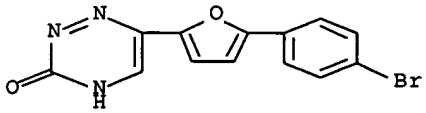
CN 3(2H)-Pyridazinone, 6,6'-(2,5-thiophenediyl)bis- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1977:165774 CAPLUS Full-text
DN 86:165774
TI Effect of arylfuran derivatives on the activity of pyridoxal enzymes
AU Fadeeva, N. I.; Gus'kova, T. A.; Pershin, G. N.; Degtyareva, I. N.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (1976), 10(12), 21-6
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
GI



AB Of 27 arylfuran derivs. tested, 5-(p-chlorophenyl)-2-bromoacetylfuran (I) [39170-34-8] was the most active antimicrobial agent against common bacterial and fungal species in vitro and the strongest inhibitor of aspartate aminotransferase (EC 2.6.1.1) (AST) [9000-97-9] and alanine aminotransferase (EC 2.6.1.2) (ALT) [9000-86-6]. Its p-nitro analog [39170-35-9] did not inhibit the pyridoxal enzymes and showed only weak bacteriostatic and fungistatic activities. 5-(P-bromophenyl)furyl-2- glyoxal [42142-86-9] showed strong antimicrobial and AST-inhibitory activities but did not inhibit ALT. Mercapto-containing arylfurans showed weak enzyme-inhibitory and antimicrobial activities, but thiazole, pyrrocoline, and imidazopyridine derivs. were inactive. Some of the 5-aryl-2-bromobutyl(propionyl)furan derivs. showed weak antimicrobial activity but did not affect the pyridoxal enzymes, suggesting an effect on other enzymic systems. Use of the aminotransferases is suggested in primary screening of arylfuran compds. for antimicrobial activity.
IT 62530-40-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal and fungicidal activities of, aminotransferase activity in relation to)
RN 62530-40-9 CAPLUS
CN 1,2,4-Triazin-3(2H)-one, 6-[5-(4-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)



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=> s l4 not l5
L6            2 L4 NOT L5

=> dis  1-2 bib abs

L6   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2006:163781  CAPLUS Full-text
DN   144:400522
TI   Synthesis and characterization of new fluorescent two-photon absorption
     chromophores
AU   Huang, Ping-Hsin; Shen, Jiun-Yi; Pu, Shin-Chien; Wen, Yuh-Sheng; Lin,
     Jiann T.; Chou, Pi-Tai; Yeh, Ming-Chang P.
CS   Institute of Chemistry, Academia Sinica, Taipei, Taiwan
SO   Journal of Materials Chemistry (2006), 16(9), 850-857
     CODEN: JMACEP; ISSN: 0959-9428
PB   Royal Society of Chemistry
DT   Journal
LA   English
AB   Dipolar and quadrupolar type two-photon absorption (TPA) compds. were
     synthesized and TPA cross sections (σ) were measured by Ti:sapphire
     femtosecond laser excitation fluorescence (λ = 800 nm). Among them, [2,5-bis-
     [5-(4-diphenylaminophenylethynyl)thiophen-2-yl]- [1,3,4]oxadiazole], 12, was
     structurally characterized by x-ray crystallog. The resulting data indicate
     that the structure of this compound possesses excellent coplanarity. The
     compds. have arylamines as the donor, and [1,3,4]oxadiazolyl, cyanovinyl or
     pyridazin-3,6-diyl moiety as the acceptor. Variation of arylamines and
     pendant alkyl groups has a significant influence on σ values. By an
     appropriate combination of donor and acceptor, σ values of > 103 GM (10-50
     cm4s photon·mol.-1) can be achieved. One quadrupolar mol. (13) possessing an
     arylamine donor and a pyridazine acceptor has both a high σ value (1442 GM)
     and σ/MW (1.97 GM/g).
RE.CNT  71    THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6   ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:38041  CAPLUS Full-text
DN   141:260474
TI   Synthesis and biological activity of thiophene derivatives
AU   Shklyaev, Yu. V.
CS   Inst. Tekh. Khim., Ural. Otd., RAN, Perm, 614990, Russia
SO   Kislorod- i Serusoderzhashchie Geterotsikly, [Trudy Mezhdunarodnoi
     Konferentsii "Khimiya i Biologicheskaya Aktivnost Kislorod- i
     Serusoderzhashchikh Geterotsiklov"], 2nd, Moscow, Russian Federation, Oct.
     14-17, 2003 (2003), Volume 1, 472-477.  Editor(s): Kartsev, Viktor G.
     Publisher: IBS Press, Moscow, Russia.
     CODEN: 69EZN9; ISBN: 5-902545-01-3
DT   Conference
LA   Russian
OS   CASREACT 141:260474
AB   A series of 2-thienylglyoxylic esters RCOCO2Et (R = substituted 2-thienyl) was
     synthesized by either Friedel-Crafts acylation of thiophenes with Et oxalyl
     chloride or reaction of thiophene Grignard reagents with di-Et oxalate. The
     antimicrobial activity of thiosemicarbazones of these esters and of
     trimethylammonium-functionalized hydrazides of acetyl thiophenes was studied.

=> log y
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
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STN INTERNATIONAL LOGOFF AT 13:05:12 ON 25 SEP 2006